LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.756	3	6	17	rVB	3096582	4710984	74.70%	7.665%
2	1.904	17	19	40	rVB	2599108	4998848	79.27%	8.133%
3	2.167	40	42	59	rVB3	89763	287444	4.56%	0.468%
4	5.082	293	297	307	rVB	1577905	2344797	37.18%	3.815%
5	5.493	329	333	335	rBV	5585540	6178871	97.98%	10.053%
6	6.510	419	422	425	rBV	4237740	6306195	100.00%	10.260%
7	6.647	431	434	437	rBV	4717620	5711390	90.57%	9.292%
8	6.876	452	454	457	rBV	1001641	1192730	18.91%	1.941%
9	7.036	466	468	471	rVB	3937039	4133059	65.54%	6.724%
10	7.447	500	504	506	rBV	3604397	4044319	64.13%	6.580%
11	8.168	564	567	569	rBV	1814818	1636391	25.95%	2.662%
12	9.242	658	661	664	rBV	4372210	5093191	80.76%	8.286%
13	9.631	693	695	698	rVB	315746	426513	6.76%	0.694%
14	9.916	718	720	722	rBV	1343818	1428059	22.65%	2.323%
15	10.362	758	759	761	rVB	93616	65847	1.04%	0.107%
16	10.705	786	789	792	rBV	3083421	3064163	48.59%	4.985%
17	10.831	798	800	805	rVB	127660	150408	2.39%	0.245%
18	11.276	838	839	841	rBV	90563	89013	1.41%	0.145%
19	11.402	848	850	852	rBV	1466547	1324463	21.00%	2.155%
20	11.711	875	877	878	rBV	74685	81709	1.30%	0.133%
21	11.939	895	897	899	rBV2	192696	272644	4.32%	0.444%
22	12.008	902	903	908	rVB2	41121	78324	1.24%	0.127%
23	12.614	954	956	958	rBV	270836	262590	4.16%	0.427%
24	12.717	963	965	968	rBV3	88351	130183	2.06%	0.212%
25	12.842	973	976	977	rBV	233270	293758	4.66%	0.478%
26	12.991	986	989	991	rBV	4249916	3825938	60.67%	6.225%
27	13.368	1017	1022	1023	rBV2	26493	63332	1.00%	0.103%
28	13.665	1046	1048	1051	rBV	32925	63932	1.01%	0.104%
29	13.894	1065	1068	1070	rBV	151433	242163	3.84%	0.394%
30	14.031	1078	1080	1082	rBV	1018567	1445764	22.93%	2.352%
31	14.900	1154	1156	1159	rBV2	62171	85475	1.36%	0.139%
32	15.060	1168	1170	1175	rBV	130388	264532	4.19%	0.430%
33	15.357	1194	1196	1198	rBV	91231	110799	1.76%	0.180%
34	15.414	1199	1201	1203	rBV	87814	116516	1.85%	0.190%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.483	1204	1207	1209	rVV	683053	939656	14.90%	1.529%

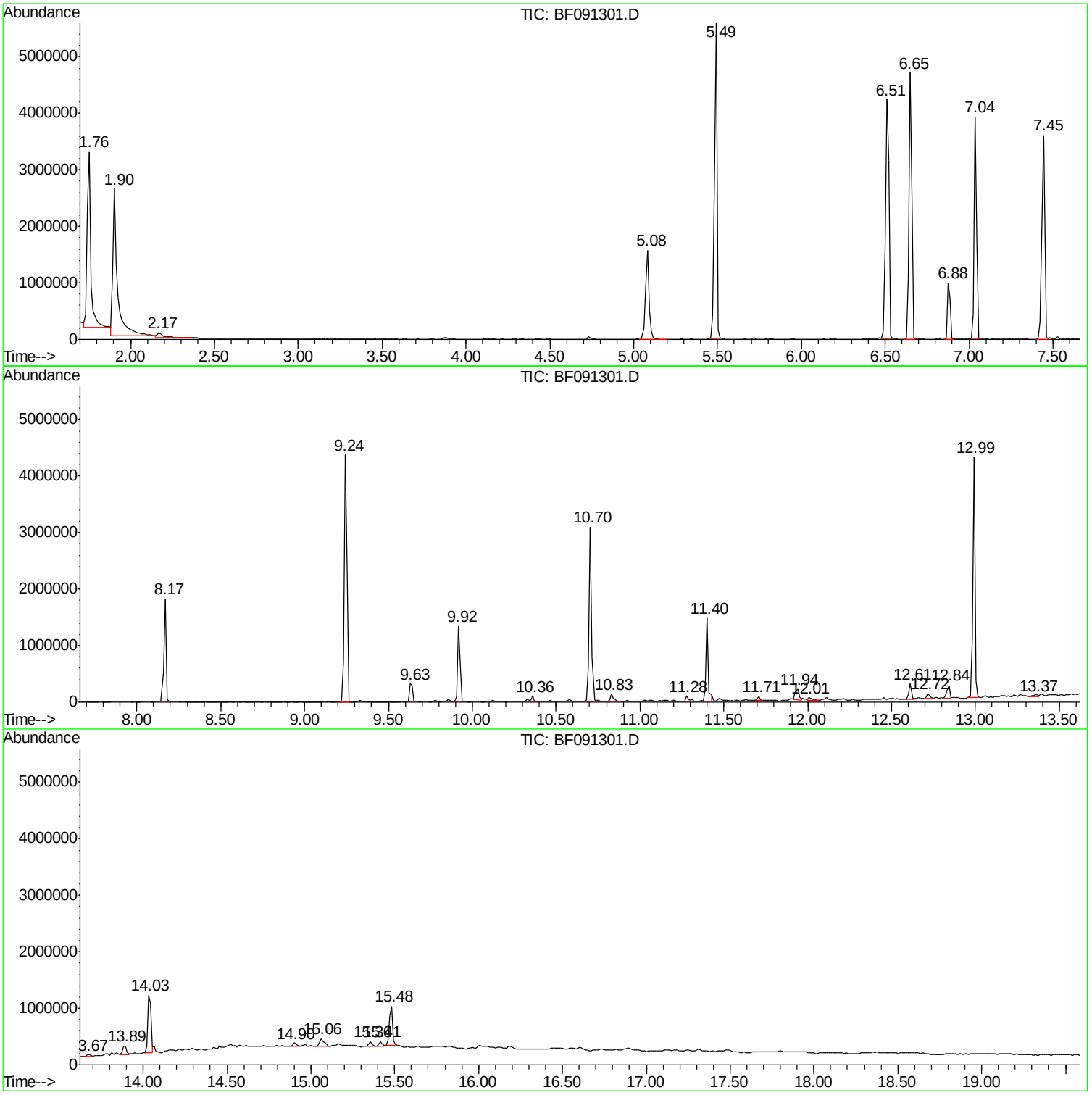
Sum of corrected areas: 61464000

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

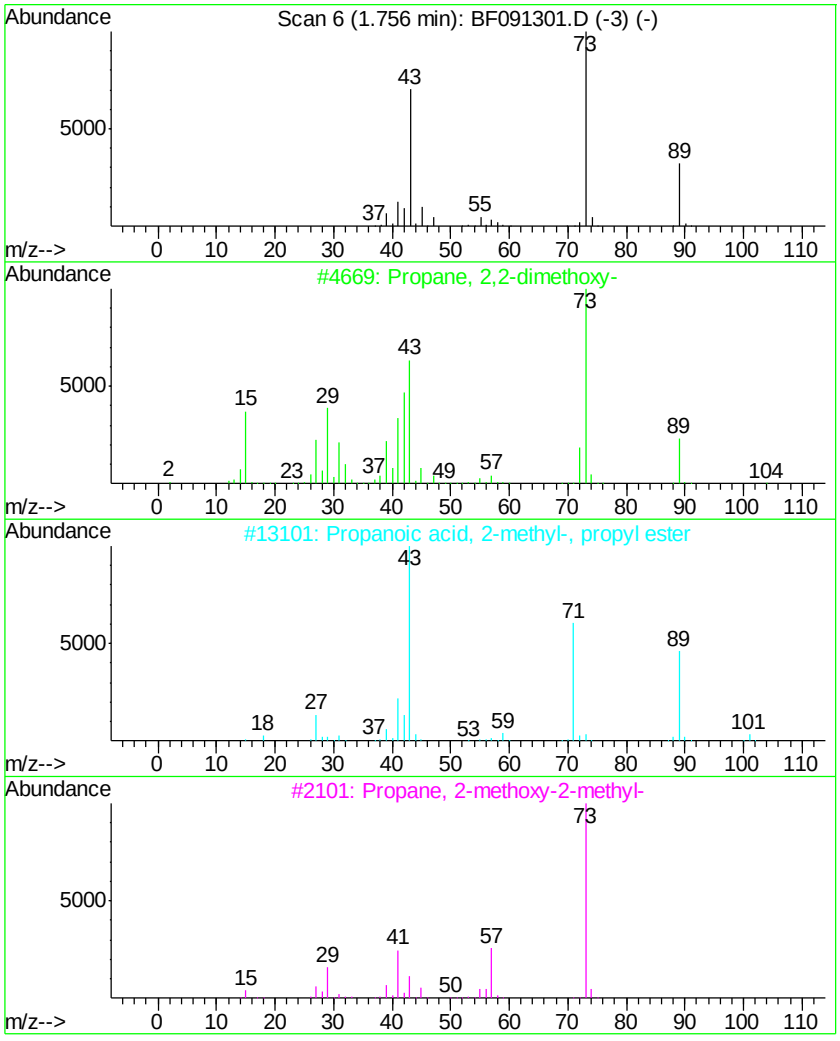
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

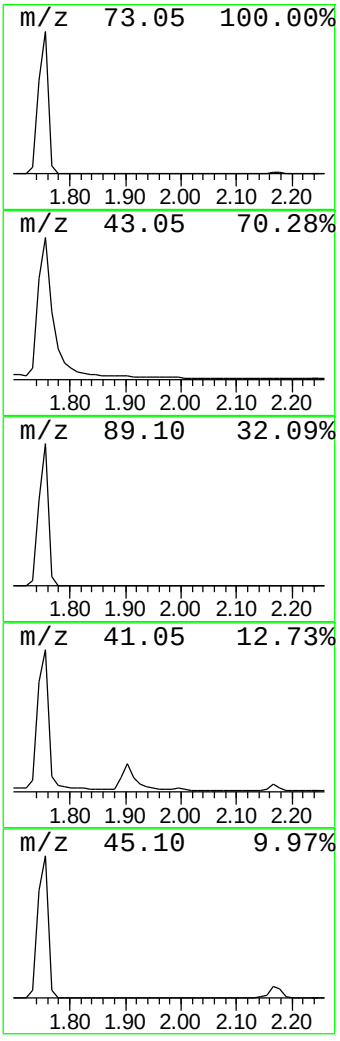
****

Peak Number 1 unknown1.76 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	79.00 ng	4710980	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	23
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

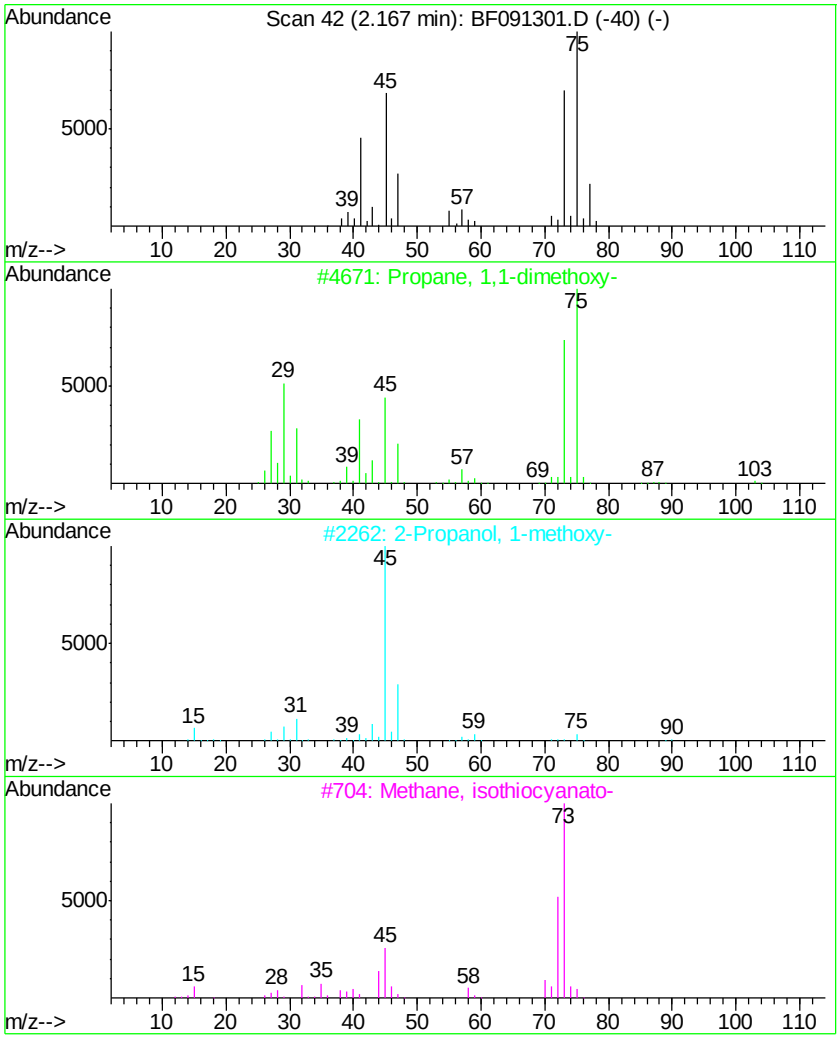
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

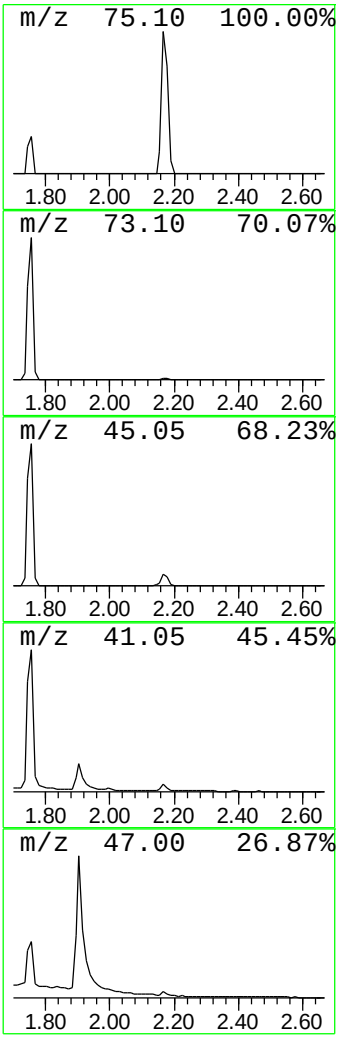
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	4.82 ng	287444	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2	2-Propanol, 1-methoxy-	90	C4H10O2	000107-98-2	23
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	22
4	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9
5	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

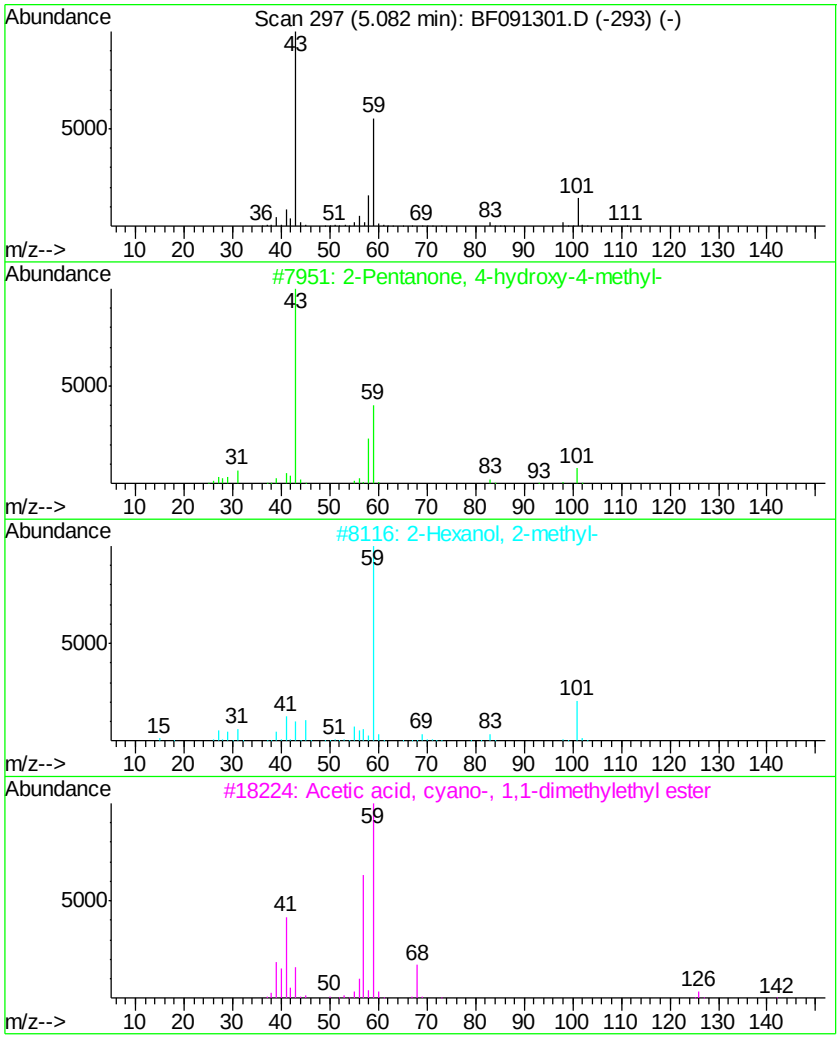
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

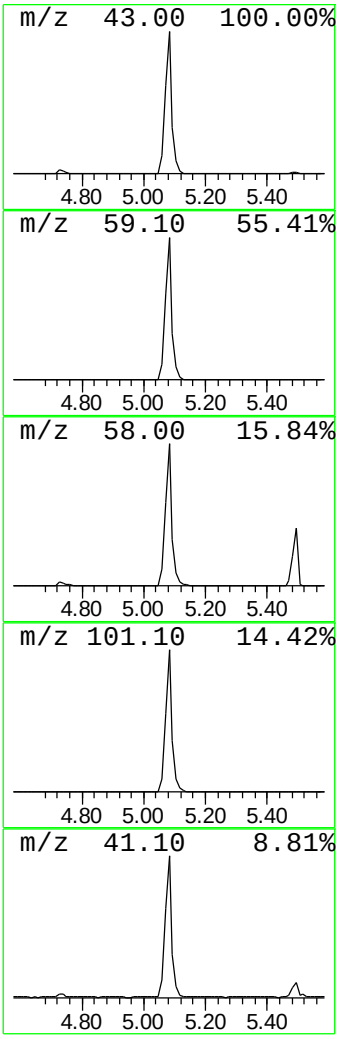
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	39.32 ng	2344800	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

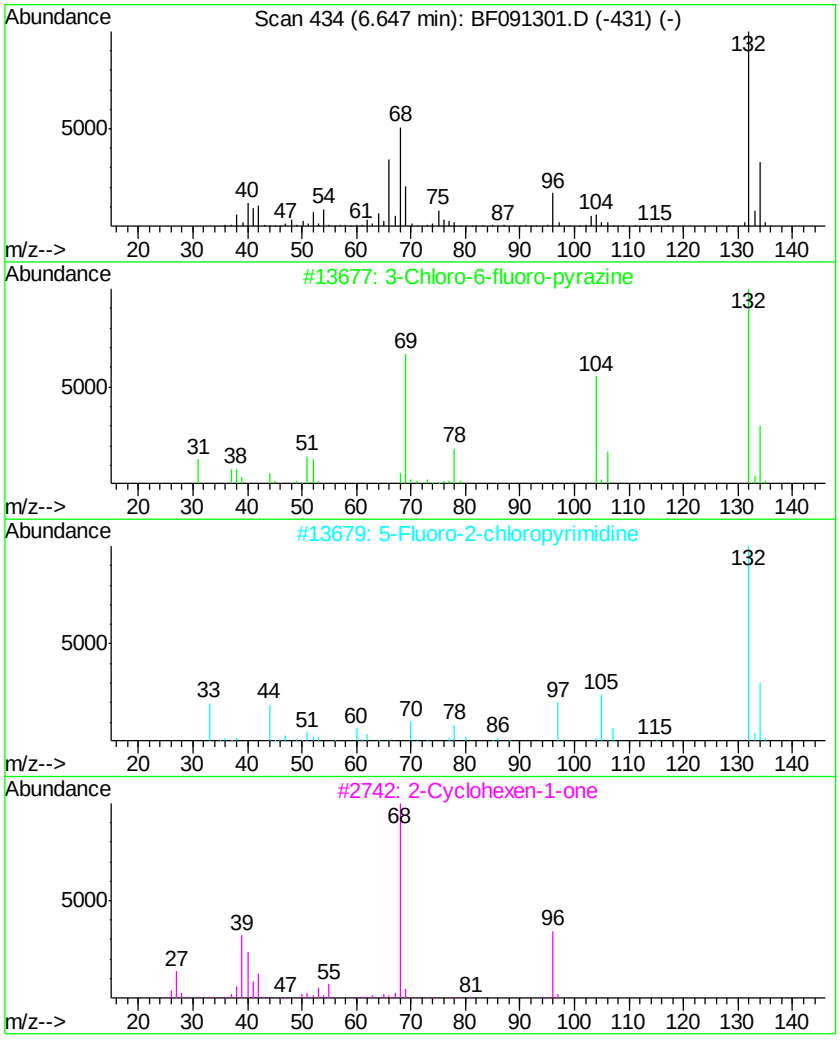
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

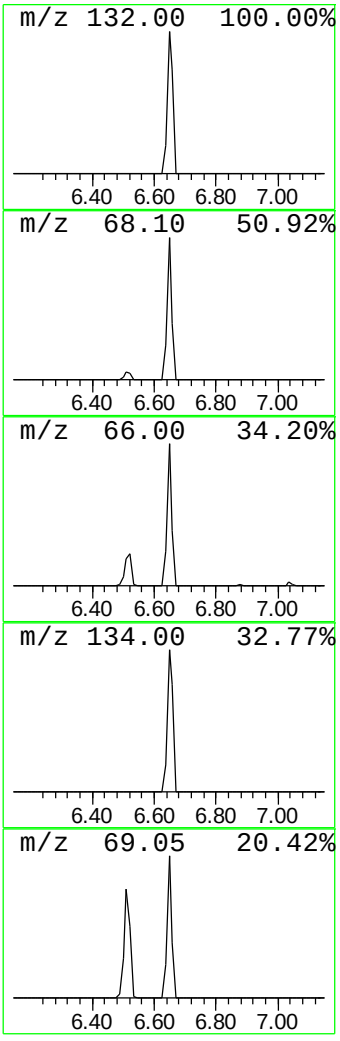
****

Peak Number 5 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	95.77 ng	5711390	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

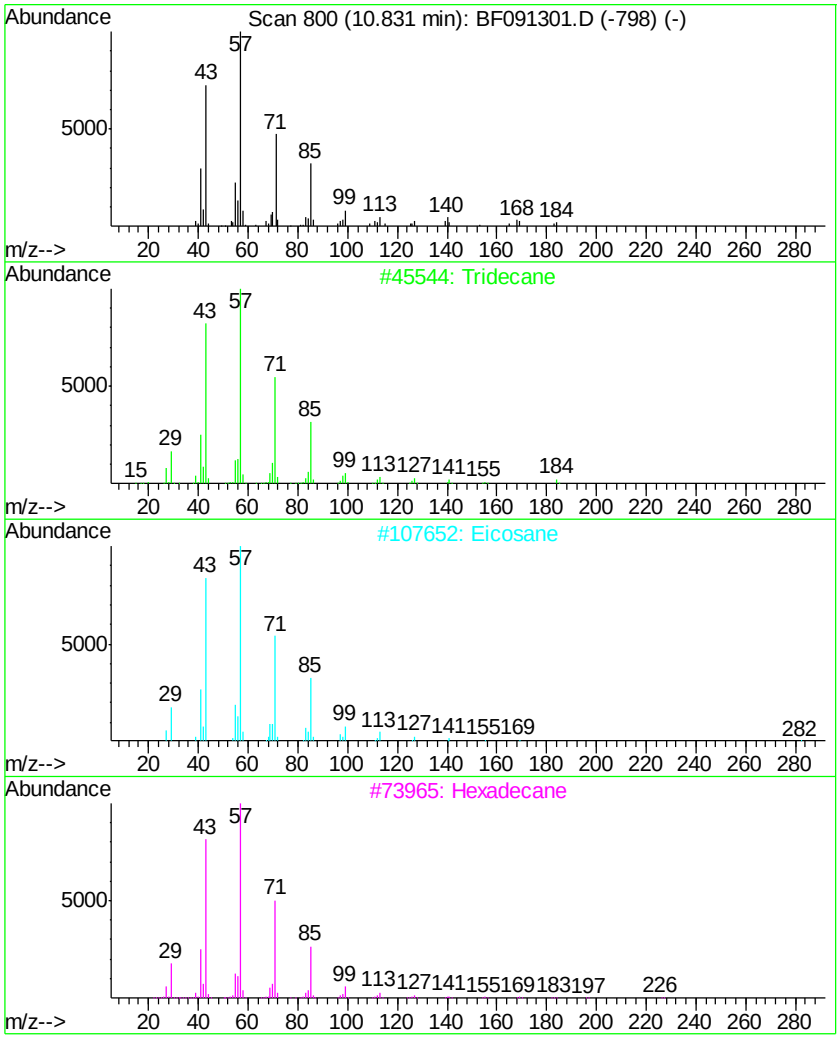
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

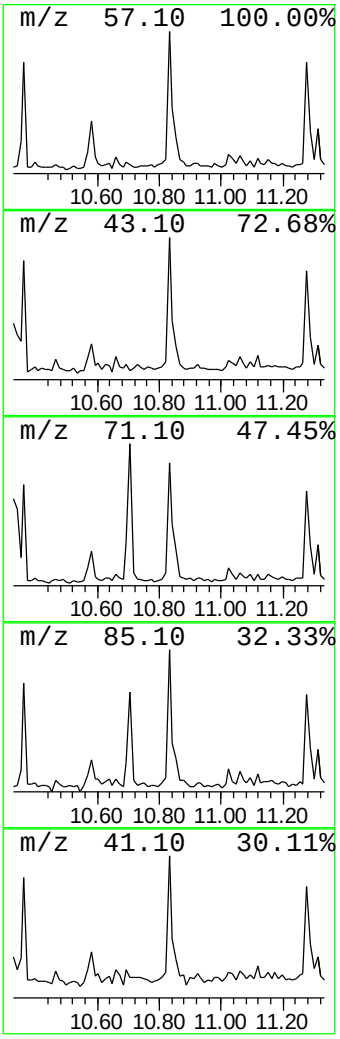
****

Peak Number 7 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	2.27 ng	150408	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Eicosane	282	C20H42	000112-95-8	90
3	Hexadecane	226	C16H34	000544-76-3	87
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

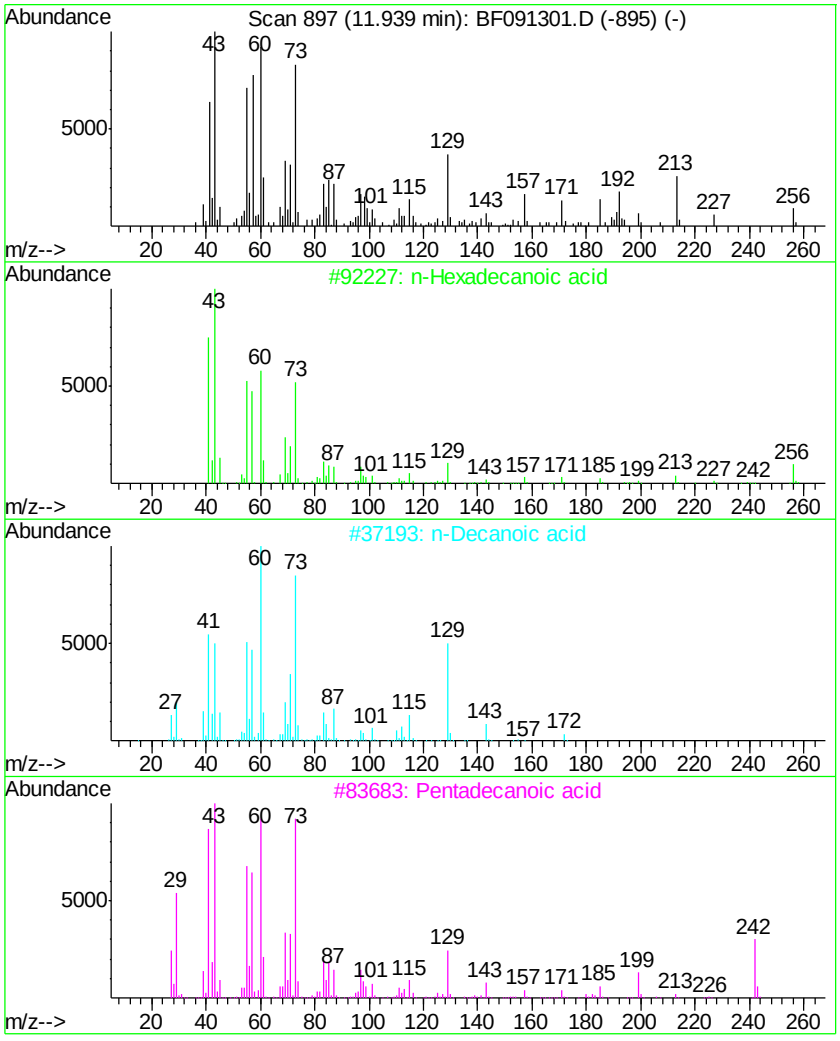
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

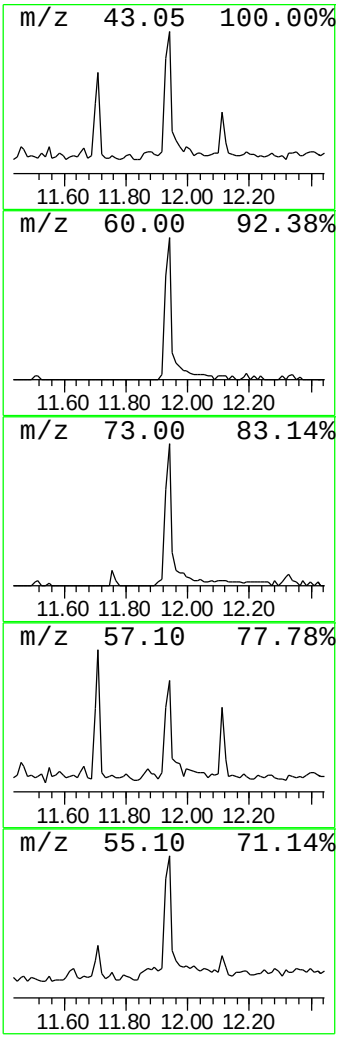
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	4.12 ng	272644	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	n-Decanoic acid	172	C10H20O2	000334-48-5	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

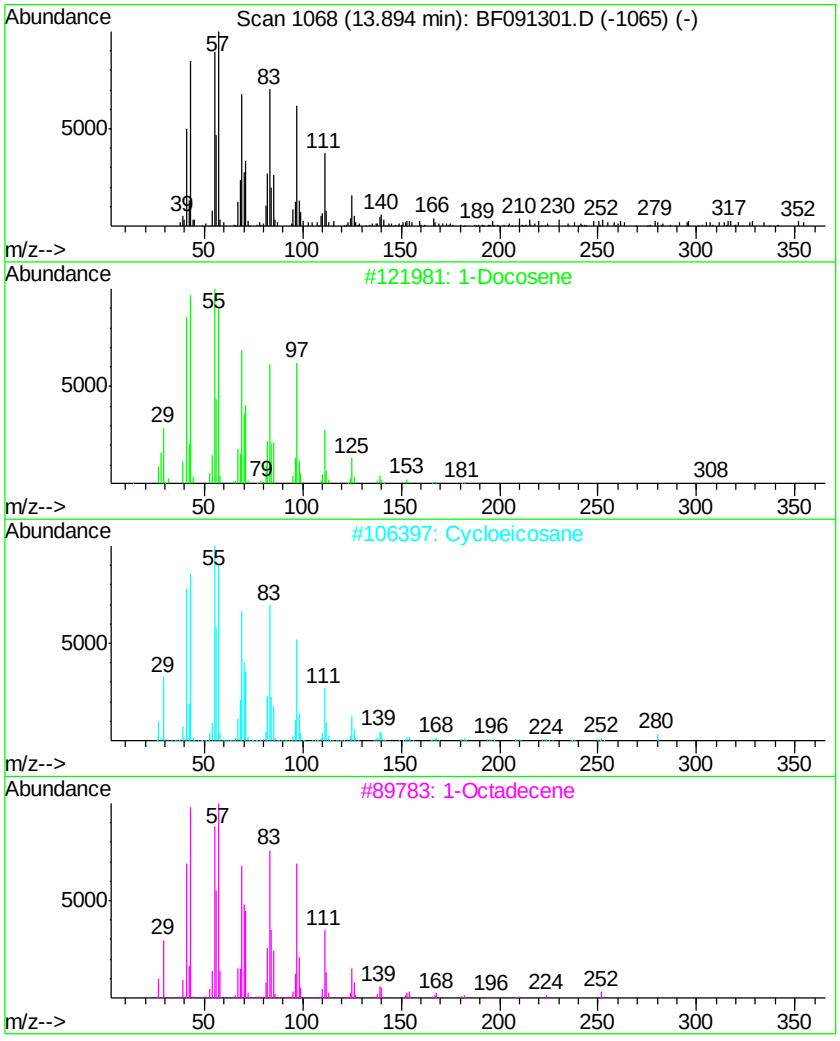
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

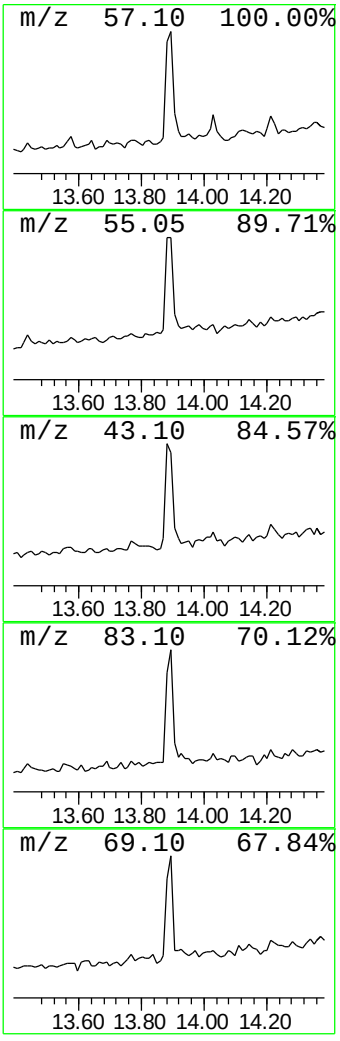
****

Peak Number 9 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	3.35 ng	242163	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Cycloeicosane	280	C20H40	000296-56-0	94
3	1-Octadecene	252	C18H36	000112-88-9	94
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
5	Cyclotetracosane	336	C24H48	000297-03-0	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

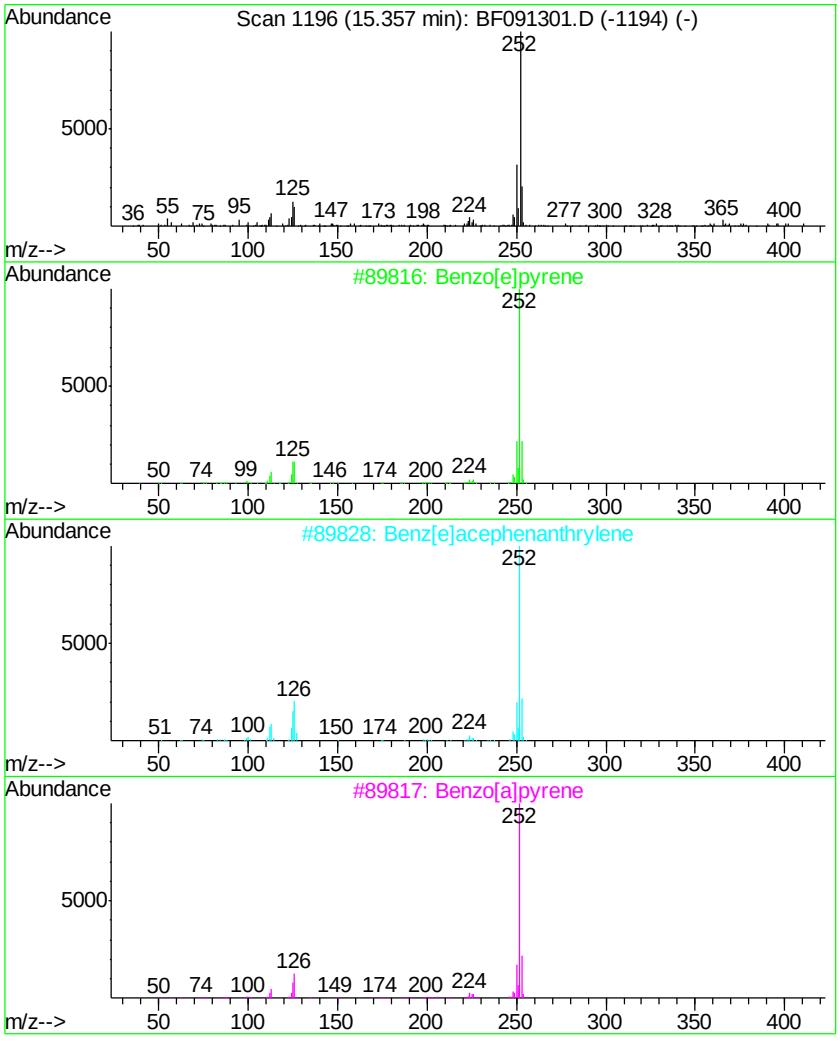
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

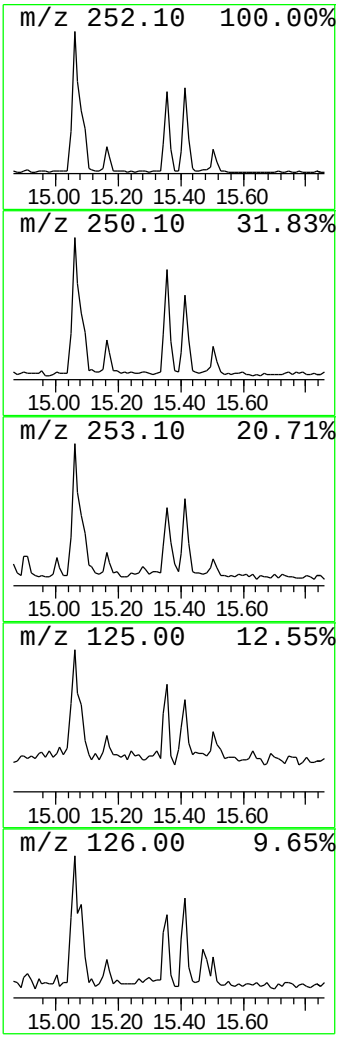
****

Peak Number 10 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.36 ng	110799	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	90
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5	Perylene	252	C20H12	000198-55-0	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091301.D
Acq On : 24 Nov 2016 3:23
Operator : UM/SJ
Sample : H5749-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GRID-MM4-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.76	1.76	79.0	ng	4710980	1	6.88	1192730	20.0
Propane, 1,1-dime...	2.17	4.8	ng	287444	1	6.88	1192730	20.0
2-Pentanone, 4-hy...	5.08	39.3	ng	2344800	1	6.88	1192730	20.0
unknown6.65	6.65	95.8	ng	5711390	1	6.88	1192730	20.0
Tridecane	10.83	2.3	ng	150408	4	11.40	1324460	20.0
n-Hexadecanoic acid	11.94	4.1	ng	272644	4	11.40	1324460	20.0
1-Docosene	13.89	3.4	ng	242163	5	14.04	1445760	20.0
Benzo[e]pyrene	15.36	2.4	ng	110799	6	15.48	939656	20.0